PB86-164886

Influence of Organic Cosolvents on Sorption of Hydrophobic Organic Chemicals by Soils

Florida Univ., Gainesville

Prepared for

Robert S. Kerr Environmental Research Lab.
Ada, OK

1985

U.S. Department of Commerce
National Technical Information Service

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA/600/J-85/293	2.	3. PB86-164886
4. TITLE AND SUBTITLE INFLUENCE OF ORGANIC CO-SOLVENTS ON SORPTION OF HYDROPHOBIC ORGANIC CHEMICALS BY SOILS (Journal Version)		5. REPORT DATE 1985 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) P. Nkedi-Kizza, P.S.C. Rao, and A.G. Hornsby		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Soil Science Department University of Florida Gainesville, FL 32611		10. PROGRAM ELEMENT NO. CBPC1A 11. CONTRACT/GRANT NO. CR-806744
12. SPONSORING AGENCY NAME AND ADDRESS Robert S. Kerr Environmental Research Lab. - Ada, OK Office of Research and Development U.S. Environmental Protection Agency Ada, OK 74820		13. TYPE OF REPORT AND PERIOD COVERED 14. SPONSORING AGENCY CODE EPA/600/15

15. SUPPLEMENTARY NOTES

Published in JOURNAL OF ENVIRONMENTAL SCIENCE AND TECHNOLOGY, 19(10):975-979, 1985

16. ABSTRACT

Sorption of anthracene and two herbicides (diuron and atrazine) by soils from aqueous solutions and binary solvent mixtures consisting of methanol-water and acetone-water was measured. These data were used to evaluate recently proposed solvophobic theory for describing sorption of hydrophobic molecules from mixed solvents. As predicted by the theory, the sorption coefficient (K^m) decreased exponentially with increasing fraction of the organic cosolvent (f^c) in the binary solvent mixtures. The slope of the ln K^m vs. f^c plot, designated as σ^c, was unique to each sorbate-solvent combination and was independent of the soil (sorbent). Thus, the organic cosolvent effects on sorption could be specified by a single parameter that combines the coefficients characterizing solvent and sorbate properties.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS (This Report) UNCLASSIFIED 20. SECURITY CLASS (This page) UNCLASSIFIED	21. NO. OF PAGES 7 22. PRICE

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

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EPA/600/J-85/293
JOURNAL ARTICLE

Influence of Organic Cosolvents on Sorption of Hydrophobic Organic Chemicals by Soils

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■ Sorption of anthracene and two herbicides (diuron and atrazine) by soils from aqueous solutions and binary solvent mixtures consisting of methanol–water and acetone–water was measured. These data were used to evaluate recently proposed solvophobic theory for describing sorption of hydrophobic molecules from mixed solvents. As predicted by the theory, the sorption coefficient (K^m) decreased exponentially with increasing fraction of the organic cosolvent (f^c) in the binary solvent mixtures. The slope of the ln K^m vs. f^c plot, designated as σ^c, was unique to each sorbate–solvent combination and was independent of the soil (sorbent). Thus, the organic cosolvent effects on sorption could be specified by a single parameter that combines the coefficients characterizing solvent and sorbate properties. The σ^c value was shown to be directly proportional to the solvent–sorbate interfacial free energy ($\Delta\gamma^c$) and the hydrocarbonaceous molecular surface area (HSA) of the sorbate.

Introduction

Most of the current data for hydrophobic organic chemicals (HOC) deal with sorption from aqueous solutions (*1–3*). However, under waste disposal and land treatment sites, it is likely that the soil solution will consist of a mixture of water and various water-miscible organic solvents. Thus, it is necessary to characterize HOC sorption by soils, not only from aqueous solutions but also from aqueous–organic mixed solvents. Only a few experimental studies to date have focused on sorption from organic solvents and solvent mixtures (*4–7*). In a recent paper, Rao et al. (*8*) have presented a theoretical approach for describing the effects of organic cosolvents on HOC sorption and used a limited amount of published data, mostly for solute retention in reversed-phase chromatographic columns, for a preliminary evaluation of the model. We report here the results from a series of experiments that were conducted to measure HOC sorption by soils from binary solvent mixtures. These data were used to evaluate the sorption model proposed by Rao et al. (*8*).

Theory

The solvophobic approach presented by Rao et al. (*8*) is based upon the reciprocal relationship between mole-fraction solubility (X) and the sorption coefficient (K). They have extended earlier theories developed for solubility and sorption in aqueous solutions (*9*, *10*) to mixed-solvent systems. Yalkowsky et al. (*9*) have shown that the solubility of a hydrophobic molecule in aqueous and binary mixed solvents are related (eq 1):

$$\ln X^m = \ln X^w + \sigma^c f^c \tag{1}$$

where

$$\sigma^c = [\Delta\gamma^c\mathrm{HSA} + \Delta\epsilon^c\mathrm{PSA}]/(kT) \tag{2}$$

The terms used in eq 1 and 2 and in other equations in this paper are defined under Glossary. The relationship between sorption coefficient K^w normalized with organic carbon content (OC) of the sorbent and the mole-fraction aqueous solubility (X^w) is expressed as (*10*)

$$\ln (K^w/\mathrm{OC}) = -\alpha \ln X^w - \frac{\Delta S_f(T^* - T)}{RT} - \beta \tag{3}$$

Rao et al. (*8*) have extended eq 3 for binary solvent systems (water plus water-miscible organic cosolvent) to yield

$$\ln (K^m/\mathrm{OC}) = -\alpha \ln X^m - \frac{\Delta S_f(T^* - T)}{RT} - \beta \tag{4}$$

Substituting eq 1 for ln X^m in eq 4 gives

$$\ln (K^m/K^w) = -\alpha\sigma^c f^c \tag{5}$$

When hydrophobic interactions are dominant in the system (i.e., $\Delta\gamma^c\mathrm{HSA} \gg \Delta\epsilon^c\mathrm{PSA}$) eq 2 simplifies to

$$\sigma^c = \Delta\gamma^c\mathrm{HSA}/(kT) \tag{6}$$

From eq 5 it is evident that the relative sorption coefficient (K^m/K^w) decreases exponentially as the fraction of organic cosolvent (f^c) increases. Also, from eq 6, at a given temperature (T) the parameter σ^c is dependent only on the sorbate and solvent properties (HSA and $\Delta\gamma^c$) and not on the sorbent characteristics. Thus, the value of σ^c for a sorbate (HOC) estimated from data for different sorbents (soils) is expected to be constant if the model assumptions are valid.

Table I. Physical and Chemical Properties of Soils

soil	mechanical analysis, % sand	silt	clay	pH[a]	OC, %	CEC, mequiv/100 g	major clay size minerals
Webster	55	20	25	7.3	3.9	21.8	smectites
Sharpsburg	6	59	35	5.6	1.8	27.0	smectites
Grenada	27	66	7	5.7	0.8	5.5	smectites
Cecil	77	17	6	5.6	0.9	3.4	kaolinite + Fe oxides
Eustis	94	3	3	5.7	0.6	1.8	quartz

[a] Measured in a 1:1 soil paste in 0.01 N $CaCl_2$.

Experimental Section

Soils. Five soils used in this study were the following: Cecil loamy sand (Typic Hapludults), Grenada silty loam (Glossic Fragiudalfs), Eustis fine sand (Typic Quartzipsamments), Sharpsburg silty clay loam (Typic Aquiudolls), and Webster silty clay loam (Typic Haplaquolls). Selected properties of these soils are shown in Table I. The above soils were chosen not only because they represent a broad spectrum of textural classes and physical–chemical properties but also because these same soils have been used in earlier studies on sorption, degradation, and leaching of pesticides (*11*, *12*).

Solvents and Sorbates. The binary solvents used in this study were various mixtures of methanol–water and acetone–water. Methanol and acetone were used because they are completely miscible in water and are expected to be found in most waste streams from industrial wastes. These two organic solvents also represent two extreme

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Table II. Some Properties of the Solvents Used[a]

solvent	boiling point, °C	viscosity,[b] cP	surface tension,[b] dyn/cm	density,[b] g/cm³	Rohrschneider[b] polarity index	refractive index	dipole moment, D	dielectric constant[b]
water	100	0.89	73	1.0	9.0	1.333	1.84	80.0
methanol	65	0.54	22	0.79	6.6	1.326	1.66	32.7
acetone	56	0.30	23	0.78	5.4	1.357	2.72	20.7

[a] Compiled from Synder (*13*). [b] At 25 °C.

Table III. Properties of Sorbates Studied

sorbate	total molecular surface area (TSA), Å²	aqueous solubility, mg/L	melting point (T^m), K	vapor pressure, mmHg
anthracene	202	7.5×10^{-2}	490	3×10^{-4}
diuron	219	4.2×10^{1}	431	2×10^{-6}
atrazine	219	3.3×10^{1}	449	3×10^{-7}

classes of polarity. Methanol is a proton donor, while acetone is a proton acceptor (*13*). Additional properties of methanol and acetone are listed in Table II.

Anthracene and two herbicides, diuron [3-(3,4-dichlorophenyl)-1,1-dimethylurea] and atrazine [2-chloro-4-(ethylamino)-6-(isopropylamino)-*s*-triazine], were selected for the sorption study. These chemicals have a wide range in aqueous solubilities, melting points, and vapor pressures (Table III). The two herbicides were used as benchmark chemicals since a large amount of sorption data are available for these chemicals (*11, 12, 14*). Anthracene was selected to represent an ideal hydrophobic sorbate without any polar functional groups, such that its total and hydrocarbonaceous surface areas (TSA and HSA, respectively) are identical. Because both diuron and atrazine have various polar functional groups, their HSA < TSA. Unfortunately, at this time, independent procedures for estimating the HSA for such polar molecules are not available. The TSA values for these three sorbates were computed by using the Hermann model (*15*) and are shown in Table III.

All organic solvents used were of high-performance liquid chromatography (HPLC) grade. The ^{12}C chemicals were EPA standards (99.9% purity), and ^{14}C-labeled compounds were purified with thin-layer chromatography (TLC) and autoradiography techniques before use.

Sorption Experiments. Equilibrium sorption isotherms were measured by using the batch slurry method (*11, 16*). For each soil–sorbate combination, sorption isotherms were measured in aqueous solutions (with 0.01 N $CaCl_2$ as the supporting electrolyte solution) as well as in various mixtures of methanol–water and acetone–water. All solutions were spiked with the appropriate ^{14}C-labeled compound to give specific activities of about 0.2 μCi/mL for anthracene and 10 μCi/L for the two pesticides. The soil:solution ratios used varied from 1:1 for aqueous solutions to 2:1 for mixed solvents. The higher soil:solution ratio was used to improve the precision of sorption measurements (*17*) as the amount sorbed was expected to decrease exponentially with increasing fraction cosolvent (*8*). Equilibrium was achieved by shaking the soil with the HOC solution in Pyrex centrifuge glass tubes for 24 h. Preliminary experiments had indicated that there was no measurable increase in HOC sorption beyond 24 h. Following equilibration, the tubes were centrifuged for 20 min at 10000 rpm (3580*g*), and the ^{14}C activity in 1-mL aliquots of the supernatant solution was assayed by liquid scintillation counting (Scinti-Verse^{R} II scintillation liquid, Fisher Scientific Co.). Decreases in HOC solution concentration were attributed to sorption by the soil. All sorption experiments were performed at a constant temperature (25 ± 1 °C).

Owing to the low aqueous solubility of anthracene and the possibility of anthracene sorption on centrifuge tube walls, the batch slurry method was modified. The amount of anthracene sorbed on the soil was directly determined by combusting a dry subsample of the soil at the end of the equilibration period. The soil sample was combusted in a Packard Tricarb Model 306B sample oxidizer, trapping the evolved CO_2 in a scintillation solution and quantifying $^{14}CO_2$ by liquid scintillation techniques. The solution concentration of [^{14}C]anthracene was determined as previously described after centrifugation.

Analysis of Sorption Data. The sorption data were fitted to the Freundlich equation $S = KC^N$. For each solvent mixture, the K values obtained for a given sorbate–soil combination were fitted to eq 5, and the value of σ^c was determined. Also, the values of relative sorption coefficients (K^m/K^w) were calculated and plotted vs. f^c for each sorbate–solvent combination. From these pooled sorption data for all soils, the σ^c value was determined by fitting eq 5 to the experimental data.

Results and Discussion

The validity of the solvophobic sorption model was evaluated first by measuring sorption of anthracene by soils from methanol–water and acetone–water mixtures. Note that for anthracene HSA = TSA because it is a polycyclic aromatic hydrocarbon. Anthracene sorption by soils is characterized by hydrophobic interactions (*9, 10*). For this reason, anthracene would serve as an ideal sorbate for evaluating the theory.

The dependence of K^m on f^c for anthracene sorption by four soils from methanol–water mixtures is shown in Figure 1A. As predicted by the theory (eq 5), a log-linear relationship describes the data over the entire range of $0 \leq f^c \leq 1$. The slopes of the lines in Figure 1A are essentially the same, indicating that the σ^c value is independent of the sorbent as predicted by eq 5. In Figure 1B the dependence of K^m on f^c for sorption of anthracene from acetone–water mixtures is shown. The data in this case show a deviation from the log-linear relationship for $f^c > 0.25$. A specific cause for the deviation has not yet been identified, though it is suspected that acetone affects the soil organic matter in some manner to alter its sorptive characteristics. Further discussion on this is presented later. It should be noted that solvent effects on sorbents were not explicitly accounted for in the model proposed by Rao et al. (*8*). The dashed lines in Figure 1B were obtained by regressing a quadratic function of the form $\ln K^m = \ln K^w + af^c + b(f^c)^2$, while the solid lines are the least-squares fit of eq 5 to the data for $f^c < 0.20$. When only the linear plots are considered, the slopes for both soils are essentially equal.

In Figure 2, the plots of the relative sorption coefficient (K^m/K^w) vs. f^c for anthracene sorption from methanol–water and acetone–water nixtures are shown. These plots

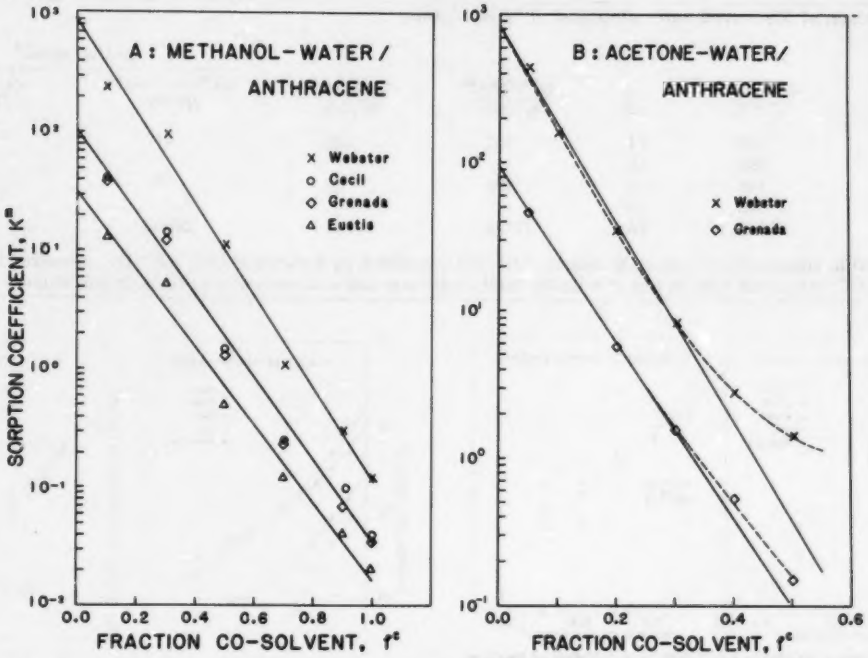

Figure 1. log-linear relationship between sorption coefficient (K^m) and fraction of organic cosolvent (f^c) for sorption of anthracene by soils from methanol–water (A) and acetone–water (B) mixtures.

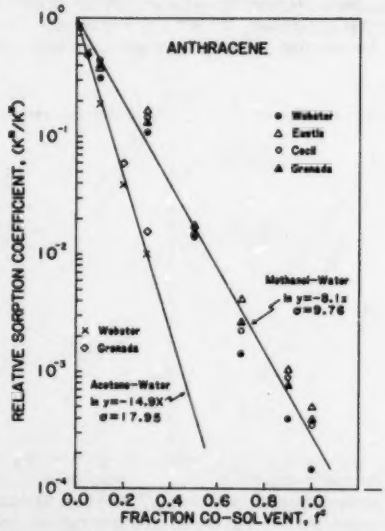

Figure 2. Relative sorption coefficient (K^m/K^w) as a function of fraction of organic cosolvent (f^c) for anthracene sorption from methanol–water and acetone–water mixtures.

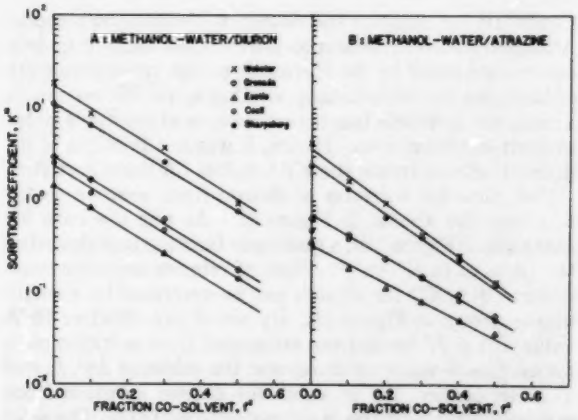

Figure 3. log-linear relationship between sorption coefficient (K^m) and fraction of organic cosolvent (f^c) for sorption of diuron (A) and atrazine (B) by soils from methanol–water mixtures.

are based on the sorption data presented in Figure 1A,B. Because of the observed nonlinearity for acetone–water mixtures, only data for $f^c < 0.3$ are included. Note that for each solvent mixture, the pooled sorption data can be described by a single line as expected from eq 5. The σ^c values estimated from these plots are 9.76 for methanol–water and 17.95 for acetone–water by using an α value of 0.83 from Karickhoff (*10*). When these σ^c values are used and when the following parameters are set at HSA = 202 (Å^2), $k = 1.38 \times 10^{-16}$ (ergs/K), and $T = 298$ (K) in eq 6, the $\Delta\gamma^c$ value for methanol–water mixture is calculated to be 1.99×10^{-15} ergs/Å^2. This value agrees closely with a value of 2.36×10^{-15} ergs/Å^2 reported by Yalkowsky et al. (*9*). The $\Delta\gamma^c$ value for the acetone–water mixture was calculated to be 3.65×10^{-15} ergs/Å^2. No published values of $\Delta\gamma^c$ for the acetone–water mixture are available at this time.

The dependence of diuron and atrazine sorption coefficients on the fraction of methanol in the binary solvent mixture is shown in Figure 3. As observed for anthracene sorption, a log-linear relationship exists between K^m and f^c for each herbicide, and the slopes of the plots for all soils are essentially the same. Therefore, plots of relative sorption coefficients (K^m/K^w) for each herbicide can be described by a single line (Figure 4). Note that because both diuron and atrazine have similar σ^c values (7.11 and 6.99, respectively), both these molecules appear to have similar "effective" HSA values. By use of these σ^c values and those of k and T given earlier, as well as $\Delta\gamma^c$ value derived from anthracene sorption data, effective HSA values of 147 and 144 Å^2 were computed for diuron and atrazine, respectively. Thus, it may be concluded that about 66% of the total molecular surface area (TSA; see

Table IV. Comparison of Measured and Calculated K^w/OC Values

sorbate	literature[a] K^w/OC	ref	calculated[b] K^w/OC	measured[c] K^w/OC	extrapolated[d] methanol–water K^w/OC	extrapolated[d] acetone–water K^w/OC
diuron	426	14	257	426	417	351
	398	18				
atrazine	146	14	204	96	90	89
	148	18				
anthracene	15849	10	17782	16032	16560	16912

[a] K^w/OC, measured in aqueous system, from literature. [b] K^w/OC, calculated by Karickhoff (*10*). [c] K^w/OC, measured in aqueous system, in this study. [d] K^w/OC, calculated with eq 5 at $f^c = 0.0$ for methanol–water and acetone–water systems, in this study.

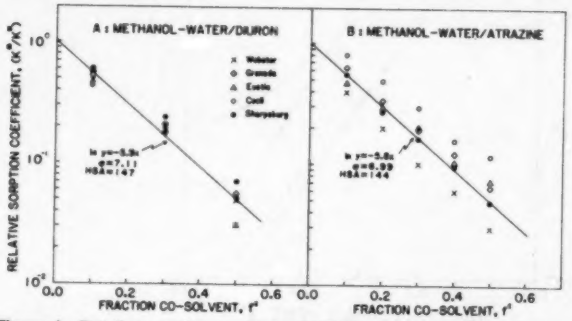

Figure 4. Relative sorption coefficient (K^m/K^w) as a function of fraction of organic cosolvent (f^c) for diuron (A) and atrazine (B) sorption from methanol–water mixtures.

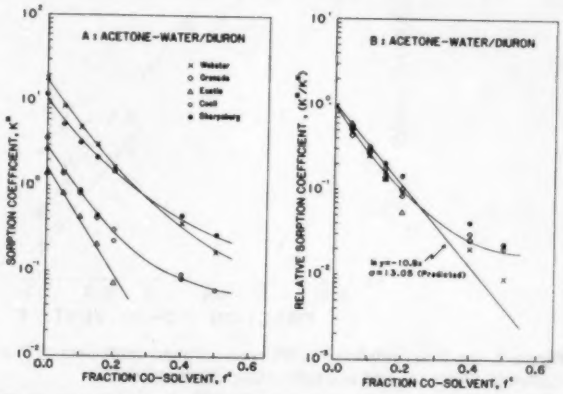

Figure 5. log-linear relationship between sorption coefficient, K^m (A), relative sorption coefficient, K^m/K^w (B), and fraction of organic cosolvent, f^c, for sorption of diuron from acetone–water mixtures.

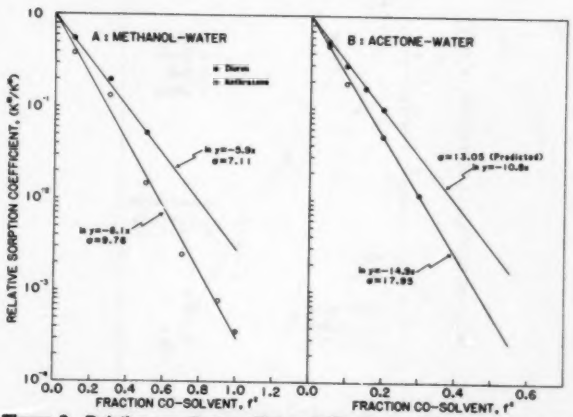

Figure 6. Relative sorption coefficient (K^m/K^w) as a function of fraction of organic cosolvent (f^c) for diuron and anthracene sorption from methanol–water (A) and acetone–water (B) mixtures.

Table III) for atrazine and diuron is hydrocarbonaceous. Although the contribution to TSA of each atom or moiety can be calculated by the Hermann model, we are unaware of the rules for determining whether a specific moiety in a complex molecule (such as diuron or atrazine) is polar or hydrocarbonaceous. Hence, it was not possible to independently estimate the HSA values for these sorbates.

The data for sorption of diuron from acetone–water mixtures are shown in Figure 5. As was the case for anthracene (Figure 1B), a quadratic function best describes the plots of ln K^m vs. f^c. Plots of relative sorption coefficients (K^m/K^w) for all soils can be described by a single line as shown in Figure 5B. By use of the effective HSA value of 147 Å^2 for diuron, estimated from sorption data for methanol–water mixtures and the values of $\Delta\gamma^c$, k, and T given earlier, the σ^c value for diuron sorption from acetone–water mixtures is estimated to be 13.05. The solid line in Figure 5B was calculated by using this σ^c value, and a reasonable agreement between measured data and the predicted line is evident for $f^c < 0.25$. Thus, we may conclude that HSA values estimated from the methanol–water system can be used to predict diuron sorption from other solvent mixtures if the $\Delta\gamma^c$ value is known. The deviation from log-linear relationship between ln K^m vs. f^c evident in Figure 5A,B further supports our suggestion that the observed deviation is due to the solvent effect on the sorbent (soil organic matter) and not likely to sorbate–solvent interactions.

The sorption data discussed above are summarized in Figure 6. The data points shown are average values for all soils, while the solid lines are calculated with eq 5 by using σ^c values discussed earlier. As predicted by the solvophobic theory (*8*), for a given solvent mixture the σ^c value is unique to each sorbate; the σ^c value increases as the sorbate HSA increases. As a further test to the effective HSA value estimated for atrazine, its sorption by Webster soil from acetone–water mixtures was measured. These data are also shown in Figure 6B. By use of the $\Delta\gamma^c$ value estimated from anthracene data, and the HSA value estimated from atrazine sorption from methanol–water mixtures, the σ^c value is computed to be 10.6. Thus, atrazine sorption from acetone–water mixtures could be predicted accurately (Figure 6B) by using model parameter values estimated from other experiments.

As noted under Experimental Section, it was difficult to measure the sorption of anthracene from aqueous solutions because of its low aqueous solubility and sorption on to container walls. The soil samples had to be combusted for a direct determination of the amount of anthracene sorbed. These problems can be overcome by measuring anthracene (and other similar solutes with low solubilities and large sorption coefficients) sorption from mixed solvents, as in this study, and extrapolating to $f^c = 0$ to estimate the K^w value. Anthracene solubility in mixed solvents is sufficiently large that sorption on container

walls was not a problem, and the amount sorbed could be estimated from the difference in initial and final solution concentrations. In Table IV the (K^w/OC) values estimated by extrapolating to $f^c = 0$ are compared with those reported in the literature and those computed by the equation proposed by Karickhoff (*10*). It is evident that the extrapolated values are in close agreement with the literature and calculated values of K^w/OC. This lends support to our suggestion that, for solutes having low aqueous solubility, K^m values should be determined in mixed solvents and then the K^w value can be estimated as shown here by using eq 5.

Summary and Conclusions

The data presented here have clearly demonstrated the validity of the solvophobic approach (*8*) for predicting the sorption of HOC from binary solvent mixtures. For each sorbate, the sorption coefficient (K^m) decreases log linearly as the fraction organic cosolvent (f^c) increases. For a given sorbate–solvent combination, the slopes of log K^m vs. f^c plots were essentially identical for all soils. Thus, the cosolvent effects on sorption could be specified by a single parameter (σ^c) that combined the characteristic of both the solvent and the sorbate. When available, independent estimates of the model parameters were used to predict the observed decrease in sorption with increasing fraction of cosolvent, as was demonstrated for sorption of anthracene from methanol–water mixtures. When literature values for the solvent and sorbate parameters could not be found, their values estimated from one solvent mixture were used to predict sorption from other solvent mixtures or for sorption of other sorbates from the same solvent mixture. The solvophobic model used here does not explicitly account for the possible effects of the solvent on the sorbent. Deviations from log-linear relation between K^m and f^c for sorption from acetone–water mixtures were attributed to such effects. Further work is warranted to understand such solvent effects. For sorbates with low aqueous solubilities, the sorption data from mixed solvents was extrapolated to $f^c = 0$ to estimate the K^w value.

Glossary

a	regression coefficient in quadratic equation
b	regression coefficient in quadratic equation
C	equilibrium solution concentration, mg/L
f^c	fraction of organic cosolvent, $0 \leq f^c \leq 1$; superscript c denotes cosolvent
g	acceleration due to gravity, cm/s^2
HSA	hydrocarbonaceous surface area, Å^2
k	Boltzmann constant, ergs/K
K	Freundlich sorption coefficient, L^N mg^{1-N} kg^{-1}
K^m	sorption coefficient in mixed-solvent systems; superscript m denotes mixed solvents, L^N mg^{1-N} kg^{-1}
K^w	sorption coefficient in water; superscript w denotes aqueous system, L^N mg^{1-N} kg^{-1}
K^m/K^w	relative sorption coefficient, dimensionless
N	Freundlich constant, dimensionless
OC	organic carbon content, g/g
PSA	polar surface area, Å^2
R	gas constant, ergs/(mol·K)
S	equilibrium sorbed concentration, mg/kg
T	ambient temperature, K
T^m	melting point, K
TSA	total molecular surface area, Å^2
X^m	mole-fraction solubility in mixed solvents
X^w	mole-fraction solubility in water
α	empirical constant
β	empirical constant
γ^w, γ^c	interfacial free energy (ergs/Å^2) at the aqueous interface and the organic cosolvent interface, respectively, with the hydrocarbonaceous surface area (HSA) of the organic molecule; superscripts w and c denote water and cosolvent, respectively.
ϵ^w, ϵ^c	interfacial free energy (ergs/Å^2) at the aqueous interface and the organic cosolvent, respectively, with the polar surface area (PSA) of the organic molecule; superscripts w and c denote water and organic cosolvent, respectively
$\Delta\gamma^c$	$\gamma^w - \gamma^c$, ergs/Å^2
$\Delta\epsilon^c$	$\epsilon^w - \epsilon^c$, ergs/Å^2
ΔS_f	entropy of fusion, ergs/(K·mol)

Registry No. Anthracene, 120-12-7; diuron, 330-54-1; atrazine, 1912-24-9; methanol, 67-56-1; acetone, 67-64-1.

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Received for review November 14, 1984. Revised manuscript received March 19, 1985. Accepted March 28, 1985. This study was supported in part by grant funds from the U.S. EPA Cooperative Agreement CR-811144. Approved for publication as Florida Agricultural Experiment Station Journal Series No. 6304.

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